

In situ X-ray and neutron diffraction studies of hcp iron hydride

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The internal structure of the Earth can be divided into a “rock mantle” and a “metallic iron core”. The mantle is mainly composed of silicate minerals, but experimental studies suggested the presence of metallic iron in the Earth’s mantle [e.g., Frost et al., 2004; Rohrbach et al., 2007]. Metallic iron has been discovered as an inclusion in diamond and peridotite originating from the deep Earth [Jones et al., 2008; Ishimura et al., 2009]. Therefore, considering that there is a metallic core below the mantle, metallic iron exists all over the deep Earth. In addition, one of the major features of the Earth is the presence of water. Water is thought to exist not only as surface seawater but also as OH ions in the deep Earth minerals. Hydrogen can be partitioned into metallic iron than silicate minerals [e.g., Shibasaki et al., 2009]. Therefore, it is expected that metallic iron existing in the deep Earth is hydrogenated.

The phase diagram changes abruptly when pure metallic iron is hydrogenated. In the case of pure metallic iron, fcc (face-centered cubic) or hcp (hexagonal closed packing) phase can be present under deep Earth conditions. On the other hand, fcc or dhcp (double hexagonal close packing) phase appears in the case of iron hydride. The hcp phase of iron hydride is a metastable phase. Conventional phase diagram of iron hydride has been determined only in experiments under hydrogen saturated conditions. However, our recent studies have revealed that hcp iron hydride is stable under low-concentration hydrogen condition [e.g., Machida et al., 2019]. Therefore, experiments under low-concentration hydrogen condition are important to discuss iron hydride under the deep Earth.

We conducted in-situ neutron diffraction experiments under high pressure and high temperature at J-PARC MLF BL11 to determine hydrogen-induced volume expansion coefficient of hcp-FeD_x. Deuterated Ammonia borane (ND₃BD₃) was used as hydrogen source. This material decomposed to D₂ and BN at high pressure and high temperature conditions. The experimental conditions were 10-12 GPa, 300-900 K. Hydrogen content was controlled to D/Fe = 0.45. In addition, we conducted in-situ X-ray diffraction experiment under high pressure and high temperature at SPring-8 BL04B1 and BL14B1 to determine P-T-x phase diagram, especially maximum hydrogen content of hcp-FeH_x at a high pressure and high temperature condition. The experimental conditions were 3-16 GPa, 300-1100 K. Hydrogen content was controlled to D/Fe = 0.5-0.8.

In the in-situ X-ray experiments, we observed coexistence of hcp and fcc-FeH_x. The hydrogen content is $x = 0.4$ and 0.7 for hcp and fcc-FeH_x at 15 GPa and 700 K, respectively. There is an immiscibility gap between hcp and fcc-FeH_x. In this presentation, we will discuss hcp iron hydride based on the results of neutron diffraction experiments.

Keywords: iron hydride, hexagonal closed packing phase, X-ray, neutron